201-15118

Safety, Health & Environment Excellence Center
1007 Market Street, DuPont 6082
Wilmington, DE 19898
302-773-0910 (Office) – 302-774-3140 (Fax)
Edwin.L.Mongan-1@usa.dupont.com

February 12, 2004

Marianne Lamont Horinko, Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 2216

Attn: Chemical Right-to-Know Program

Re: EPA comments on the Test Plan and Robust Data Summary for Hexamethyleneimine

Dear Administrator Horinko,

E. I. du Pont de Nemours & Company, Inc. received EPA's comments on the test plan and robust data summary for Hexamethyleneimine and is pleased to respond. We have considered the recommended revisions to physiochemical data, environmental fate, and ecological effects. We have revised our submittal as needed on the attached summary sheet. Also included with this submittal is a revised robust data summary.

Please feel free to contact me with any questions or concerns you may have with regards to this submission at Edwin.L.Mongan-1@usa.dupont.com or by phone at 302-773-0910.

Sincerely,

Edwin L. Mongan, III
Manager, Environmental Stewardship
DuPont Safety, Health & Environment

Cc: Charles Auer – U.S. EPA
Office of Pollution Prevention & Toxics
U. S. Environmental Protection Agency
401 M Street, SW
Washington, DC 20460

Hexamethyleneimine: Response to EPA Comments

Physiochemical Data

EPA comment: *Partition Coefficient*. While OECD allows for estimation of log Kow, in this case EPA strongly recommends that the submitter provide a measured value because water solubility is also questionable.

Response: Hexamethyleneimine has an estimated log Kow of 1.7, which is a conservative estimate in terms of partitioning into living tissue. Additionally, provided water solubility data have been supported with additional modeled values and analog information. Therefore, no testing for log Kow will be performed.

EPA comment: *Water Solubility.* The submitter provided a water solubility value taken from a computerized database (HSDB). However, EPA notes that the value given in this reference is the activity coefficient, which was incorrectly used in HSDB as a water solubility value; thus it has been incorrectly reported by the submitter. The DuPont MSDS for this material states that it is miscible with water. OECD guideline 105 requires that the water solubility be measured if it is greater than 1 µg/L. Because of these inconsistencies the submitter needs to provide measured water solubility data for this chemical following OECD guideline.

Response: The submitter respectfully offers the following information in support of the submitted value for water solubility. The EPIWIN v3.05 model value for hexamethyleneimine water solubility, 4.4×10^4 mg/L, and the HSDB value, 3.19×10^4 mg/L, are very close. In addition, activity coefficients are unitless. These observations suggest that the HSDB value is correct. Additionally, one can review analog data (for example, CAS Number: 000111-92-2, chemical name: dibutylamine, molecular formula: $C_8H_{19}N$). This compound contains a secondary nitrogen with 8 carbons (4+4, symmetrical, linear). The experimental value cited by the SRC Phys Prop Database for water solubility is 3500 mg/L at 25°C; Type: EXP; Reference: CHEM INSPECT TEST INST (1992) (http://esc.syrres.com/interkow/webprop.exe?CAS=111922). The experimental value cited for this 8-carbon, secondary amine analog again supports the submitted value as being of sufficient accuracy to be used in screening estimations for environmental fate end-points. Therefore no testing for water solubility will be performed.

Environmental Fate (photodegradation, stability in water, biodegradation, fugacity).

EPA comment: The submitter provided data showing an increase in cellular protein, and considered it a positive result for biodegradation. An increase in cellular protein is not a good indication of biodegradation because it does not provide a quantitative statement about the ultimate biodegradation of the chemical. Furthermore, the study does not provide data on the degradation of the chemical into carbon dioxide, nor does it provide data on the loss of dissolved organic carbon. Therefore, the EPA considers the study

inadequate for the purposes of the HPV challenge, and recommend the submitter provide measured ready biodegradation data following OECD Guideline 301.

Response: A Closed Bottle biodegradation test following OECD Guideline 301 was performed and the data has been added to the revised document.

Ecological Effects

EPA comment: The submitter needs to supply the missing log Kow input value used to obtain the predicted values from the ECOSAR model so that an independent evaluation can be made.

Response: Requested data were added to the robust summary.